

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 4.86×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 7.85×10^{-2}

Confidence level: 6.97×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone

Measured: 4.60×10^{-12}

Predicted: 5.97×10^{-12}

Image not found

1,3,5-Cycloheptatriene

Measured: 9.69×10^{-11}

Predicted: 1.00×10^{-10}